

The total cross section for electron capture by protons from hydrogen molecule can be found out from the formula

$$Q = 2\pi \int_0^\infty |B(\infty)|^2 p dp.$$

The value of this cross section at an incident energy of 1 keV is  $3.93 \times 10^{-16} \text{ cm}^2$ . This compares well with the recent experimental value  $\sim 4.3 \times 10^{-16} \text{ cm}^2$  obtained by Koopman (1967).

Details of our calculations and results will be published elsewhere.

The authors are thankful to Prof. D. Basu, Head of the Department of Theoretical Physics, Indian Association for the Cultivation of Science, for his kind interest and helpful comments.

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### INFRARED ABSORPTION SPECTRA OF GUAIACOL

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(Received August 14, 1968)

Though the possibility of intramolecular hydrogen bond in guaiacol molecule was not discussed by early authors (Wulf and Liddel, 1935; Pauling, 1936), Batuev (1945), Baker and Shulgin (1958) and Korotkov (1960) later commented on the possibility of existence of a weak intramolecular bond in the molecule. Richards and Walker (1961), however, observed that this bond may not be very weak.

None of these authors apparently compared the absorption spectrum of the pure liquid with the spectra of solutions. In some previous investigations on *o*-chlorophenol (Sirkar *et al.*, 1958) and *o*-bromophenol (Banerjee and Chakraborty, 1961) it was observed that in the liquid state mostly dimers formed through intermolecular bond are present. Further, it was observed in the case of hydroxy phenols (Mukherjee and Banerjee, 1967) that in strong proton accepting solvent intermolecular bond between phenols and solvent molecules takes place. In view of these facts, it was thought worthwhile to study the influence of different solvents and mixed solvent on the OH vibrational band of guaiacol and the results of such an investigation have been reported in the present note.

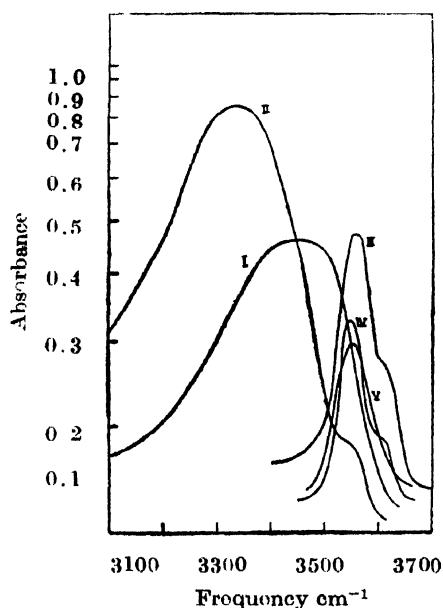


Figure 1. Infrared absorption bands of Guaiacol

- I Pure liquid (thin film)  
 II 0.01M Soln. THF  
 III " "  $\text{CHCl}_3$   
 IV " "  $\text{CCl}_4$   
 V " " benzene

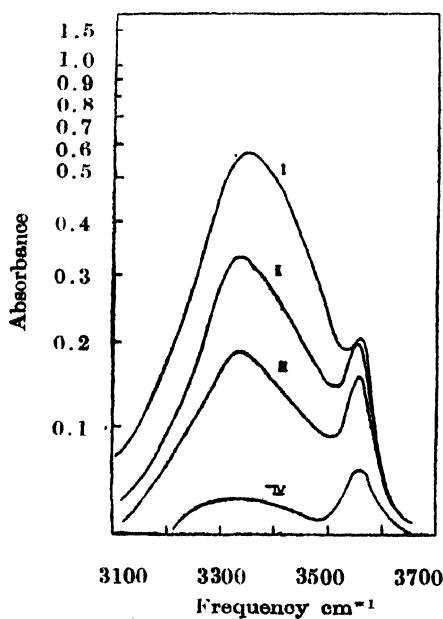


Figure 2. Infrared absorption bands of Guaiacol

- I 0.01 M Soln. of guaiacol in ether  
 II 50% soln. of I in  $\text{CCl}_4$   
 III 30% " " "  
 IV 3% " " "

The samples of guaiacol and the solvents used were of chemically pure quality and were distilled and dried before use. The spectra were recorded with a Perkin-Elmer Model 21 spectrophotometer fitted with rock salt optics. The spectra were calibrated against the absorption of atmospheric water vapour at  $3741\text{ cm}^{-1}$  and the accuracy of measurement of frequencies was about  $\pm 5\text{ cm}^{-1}$ . All measurements were made at  $26^\circ\text{C}$ .

The absorption curves are reproduced in figures 1 and 2. In the absorption curve due to thin film of liquid guaiacol a very broad band of half width of about  $250\text{ cm}^{-1}$  and having its centre at about  $3450\text{ cm}^{-1}$  is observed. This presumably represents the OH vibrational band due to dimeric molecules present in the liquid, the dimers being formed through intermolecular OH...O bond between OH groups of neighbouring molecules. In 0.01M solutions in  $\text{CCl}_4$ ,  $\text{CHCl}_3$  and  $\text{C}_6\text{H}_6$  this broad band is replaced by a sharp peak at about  $3555\text{ cm}^{-1}$  which obviously means that only single molecules are present in dilute solutions. As pointed out by Sirkar *et al* (1958) this band may not belong to *cis* configuration. In the case of 0.01M solutions in ether and tetrahydrofuran, in addition to the  $3558\text{ cm}^{-1}$  band a new intense peak at about  $3350\text{ cm}^{-1}$  appears in the absorption curve. This probably indicates that strong intermolecular hydrogen bond is formed between molecules of guaiacol and the neighbouring molecules of the respective solvent. When 0.01 M solution of guaiacol in ether is further dissolved in  $\text{CCl}_4$  in different proportions the relative intensity of the  $3352\text{ cm}^{-1}$  band with respect to that of the  $3558\text{ cm}^{-1}$  band falls off regularly on dilution in  $\text{CCl}_4$ . This clearly means that the guaiacol-ether complex gradually breaks up and more and more single molecules are formed. As pointed out in a previous communication on *o*-bromophenol (Banerjee and Chakraborty, 1961) the relative abundance of the single molecules and associated molecules may be estimated from a systematic comparison of the relative intensities of these two bands.

The authors are grateful to Prof. G. S. Kastha for his kind interest in the work.

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